NON-REAL EIGENVALUES FOR $\mathcal{PT}$-SYMMETRIC DOUBLE WELLS

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Abstract. We study small, $\mathcal{PT}$-symmetric perturbations of self-adjoint double-well Schrödinger operators in dimension $n \geq 1$. We prove that the eigenvalues stay real for a very small perturbation, then bifurcate to the complex plane as the perturbation gets stronger.

In memory of Louis Boutet de Monvel

Contents

1. Introduction

We study spectral properties of small, $\mathcal{PT}$-symmetric perturbations of self-adjoint double-well Schrödinger operators

$$P_\varepsilon = -h^2\Delta + V_\varepsilon, \tag{1.1}$$

on M, a smooth compact Riemannian manifold of dimension n, or $\mathbb{R}^n$, where the potential is of the form

$$V_\varepsilon(x) = V_0(x) + i\varepsilon W(x). \tag{1.2}$$

Here $\varepsilon \in \mathbb{R}$, $|\varepsilon| \ll 1$, $V_0, W \in \mathcal{C}^\infty(M;\mathbb{R})$ and W is bounded. Δ denotes the Laplace-Beltrami operator on M.

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The one dimensional-case has been considered in [6] under an additional assumption of analyticity, and we concentrate here on the general n-dimensional case, $n > 1$. Our new result is more general, but requires a stronger condition on the size of the perturbation parameter.

To be more precise, P_0 denotes the Friedrichs extension of the differential operator $-h^2\Delta + V_0$ from $\mathcal{C}_0^\infty(M)$. In the case $M = \mathbb{R}^n$, it is well-known that

$$\inf \sigma_{\mathrm{ess}}(P_0) \geq \liminf_{x\to\infty} V_0(x) =: \alpha, \tag{1.3}$$

or in other words, that the spectrum of P_0 in $]-\infty, \alpha[$ is purely discrete. This assertion is also true when M is a compact manifold, with $\alpha = +\infty$ in that case.

Since W is bounded, we can define $P_\varepsilon = P_0 + i\varepsilon W$ as a closed operator with the same domain as P_0, and it is proved in Proposition A.1 below that the spectrum of P_ε is discrete in the half-plane $\{z \in \mathbb{C},\ \mathrm{Re}\, z < \alpha\}$. To fix the ideas, we will assume when $M = \mathbb{R}^n$ that

$$\alpha > 0. \tag{1.4}$$

Thus there exists an h-independent neighborhood $\mathcal{E}$ of $E_0 = 0$ in $\mathbb{C}$ such that P_0 and P_ε have only discrete spectrum in $\mathcal{E}$.

We shall also assume that we have an isometry $\iota : M \to M$, different from the identity, such that

$$\iota^2 = \mathrm{id}, \tag{1.5}$$

and

$$V_0 \circ \iota = V_0. \tag{1.6}$$

We suppose further that V_0 has a double-well structure at energy $E_0 = 0$, and that the two wells are exchanged by ι. More precisely, we assume that

$$V_0^{-1}(]-\infty, 0]) = U_{-1} \cup U_1, \quad U_{-1} \cap U_1 = \emptyset, \tag{1.7}$$

where $U_{\pm 1} \subset M$ are non-empty, closed and hence compact in view of the assumption (1.4), and that

$$\iota(U_{-1}) = U_1. \tag{1.8}$$

In Section 2 we review some basic facts about the Lithner-Agmon metric $V_0(x)_+ dx^2$ (cf. (2.2)) and the corresponding distance $d(x, y)$, which may be degenerate in the sense that $d(x, y)$ may be zero when $x \neq y$, but which is symmetric and satisfies the triangle inequality (cf. (2.3), (2.4)) and is a locally Lipschitz function (cf. (2.5)–(2.7)).

Let $\mathrm{diam}_d(U_j)$ denote the diameter of U_j with respect to d. Then the two diameters are equal and we assume that

$$\mathrm{diam}_d(U_j) = 0,\ j = \pm 1. \tag{1.9}$$

To describe the spectrum of P_0, it is convenient to introduce two self-adjoint reference operators. Let $\chi_{\pm 1} \in \mathcal{C}_0^\infty(M;[0,1])$ have the following properties:

$$\chi_j = 1 \text{ near } U_j, \tag{1.10}$$

$$\operatorname{supp}\chi_j \subset B(U_j,\delta) =: U_j^\delta \tag{1.11}$$

where $\delta > 0$ is small. Here

$$B(U_j,\delta) = \{x \in M;\, d(U_j,x) < \delta\}.$$

Put

$$\widetilde{P}_j = \widetilde{P}_{0,j} = P_0 + \lambda\chi_{-j},\ \ j = \pm 1. \tag{1.12}$$

Here $\lambda > 0$ is a constant that we choose large enough so that

$$\{x \in M;\, V_0(x) + \lambda\chi_{-j}(x) \leq 0\} = U_j,$$

and hence the effect of adding $\lambda\chi_{-j}$ to V_0 is to fill the well U_{-j}. If we define

$$\mathcal{P}u = u \circ \iota,\ \ u \in L^2(M), \tag{1.13}$$

then $\mathcal{P}$ is unitary on $L^2(M)$ with $\mathcal{P} \neq 1 = \mathcal{P}^2$ and we have

$$\mathcal{P} \circ P_0 = P_0 \circ \mathcal{P}, \tag{1.14}$$

$$\mathcal{P} \circ \widetilde{P}_j = \widetilde{P}_{-j},\ \ j = \pm 1. \tag{1.15}$$

The last relation implies in particular that $\widetilde{P}_{-1}$ and $\widetilde{P}_1$ have the same spectrum.

Assume that

$$\widetilde{\mu}(h) = o(h) \tag{1.16}$$

is a simple eigenvalue of $\widetilde{P}_1$ (and hence of $\widetilde{P}_{-1}$), and that

$$\exists C_0, N_0 > 0,\ \sigma(\widetilde{P}_{\pm 1}) \cap \,]\widetilde{\mu}(h) - h^{N_0}/C_0, \widetilde{\mu}(h) + h^{N_0}/C_0[\, = \{\widetilde{\mu}(h)\}. \tag{1.17}$$

As we shall review in Section 3, if $\delta > 0$ is small enough, then for $h > 0$ small enough, P_0 has exactly two eigenvalues in the interval

$$]\widetilde{\mu}(h) - h^{N_0}/(2C_0), \widetilde{\mu}(h) + h^{N_0}/(2C_0)[,$$

namely the eigenvalues $\mu(h) \pm |t(h)|$ of the matrix in (3.8),

$$\begin{pmatrix} \mu(h) & t(h) \\ \overline{t(h)} & \mu(h) \end{pmatrix},$$

where $\mu(h) \in \mathbb{R}$, $t(h) \in \mathbb{C}$ satisfy for all $\delta > 0$,

$$\mu(h) = \widetilde{\mu}(h) + \mathcal{O}_\delta(e^{(\epsilon(\delta) - 2S_0)/h}),\ \ \epsilon(\delta) \to 0,\ \delta \to 0,$$

$$\forall \alpha > 0,\ t(h) = \mathcal{O}_\alpha(e^{(\alpha - S_0)/h}).$$

Here, the constant S_0 is the Lithner-Agmon distance between the two wells $U_{\pm 1}$:

$$S_0 = d(U_1, U_{-1}). \tag{1.18}$$

As a matter of fact, quite often we also have a lower bound on $|t(h)|$:

$$\forall \alpha > 0,\ \ |t(h)|^{-1} = \mathcal{O}_\alpha(e^{(\alpha+S_0)/h}).$$

There are nowadays a lot of precise results available on the tunneling coefficient $t(h)$. One may refer for example to [7], [4] or to the review paper [8] and the references therein.

Concserning the perturbation W, we assume also that

$$W \circ \iota = -W. \tag{1.19}$$

Then $\mathcal{P}P_\varepsilon = P_{-\varepsilon}\mathcal{P}$, where we also remark that $P_{-\varepsilon} = P_\varepsilon^*$. Now if we denote by $\mathcal{T}$ the anti-linear operator defined by

$$\mathcal{T}u(x) = \overline{u(\bar{x})}, \tag{1.20}$$

we see that $\mathcal{T}P_\varepsilon = P_{-\varepsilon}\mathcal{T}$, so that P_ε is $\mathcal{PT}$-symmetric:

$$\mathcal{PT}P_\varepsilon = P_\varepsilon\mathcal{PT}. \tag{1.21}$$

The main result of this paper is the following

Theorem 1.1.— *Under the above assumptions, the operator P_ε has exactly two eigenvalues (counted with their algebraic multiplicity) in $D(\widetilde{\mu}, h^{N_0}/C)$ for $C \gg 0$ and for ε real such that $|\varepsilon| \ll h^{N_0}$. These eigenvalues are equal to the eigenvalues of the matrix*

$$M_\varepsilon = \begin{pmatrix} a(\varepsilon) & b(\varepsilon) \\ \overline{b}(\varepsilon) & \overline{a}(\varepsilon), \end{pmatrix}$$

and hence of the form

$$\lambda_\pm = \operatorname{Re} a \pm \sqrt{|b|^2 - (\operatorname{Im} a)^2}.$$

Here $a(\varepsilon) = a(\varepsilon; h)$, $b(\varepsilon) = b(\varepsilon; h)$ satisfy,

$$a(0;h) = \mu(h), \quad b(0;h) = t(h),$$

$$\partial_\varepsilon a = i\int W(x)|e_1^0(x)|^2 dx + \mathcal{O}(\varepsilon h^{-N_0}) + \mathcal{O}_\delta(e^{(\epsilon(\delta)-2S_0)/h}),$$

$$\partial_\varepsilon b = \mathcal{O}_\delta e^{(\epsilon(\delta)-S_0)/h},$$

for all $\delta > 0$, where $\epsilon(\delta) \to 0$, $\delta \to 0$. Further, e_1^0 is the normalized eigenfunction with $(\widetilde{P}_1 - \widetilde{\mu}(h))e_1^0 = 0$.

If $W > 0$ on U_1, then

$$\int W(x)|e_1^0(x)|^2 dx \asymp 1, \tag{1.22}$$

and if we assume that (1.22) holds, then there exists $\varepsilon_+ \geq 0$ with the asymptotics,

$$\varepsilon_+ = (1 + \widetilde{\mathcal{O}}_\delta(e^{(\epsilon(\delta)-S_0)/h}))\frac{|t(h)|}{\int W(x)|e_1^0(x)|^2 dx}, \quad \epsilon(\delta) \to 0,\ \delta \to 0,$$

such that

- *The two eigenvalues are real and distinct for $|\varepsilon| < \varepsilon_+$.*
- *They are double and real when $|\varepsilon| = \varepsilon_+$.*
- *They are non-real and complex conjugate, when $\varepsilon_+ < |\varepsilon| \ll h^{N_0}$.*

2. Lithner-Agmon estimates for non-self-adjoint Schrödinger operators

We will need a few extensions of the tunneling theory in the spirit of B. Helffer and J. Sjöstrand [4] to the case of non-self-adjoint Schrödinger operators. We will follow the presentation in Chapter 6 in [3]. In the following M will denote either $\mathbb{R}^n$ or a compact Riemannian manifold. We start by reviewing exponentially weighted Lithner-Agmon estimates. The following is an immediate extension of Proposition 6.1 in [3].

Proposition 2.1.— *Let $\Omega \Subset M$ be open with smooth boundary and put $P = -h^2\Delta + V(x)$, for some fixed $V \in \mathcal{C}(\overline{\Omega};\mathbb{C})$. Let $\Phi \in \mathcal{C}^2(\overline{\Omega};\mathbb{R})$ Then for every $u \in \mathcal{C}^2(\overline{\Omega})$ with $u_{|\partial\Omega} = 0$, we have*

$$\begin{aligned} &h^2 \int_\Omega |\nabla(e^{\Phi/h}u)|^2 dx + \int_\Omega (\operatorname{Re} V(x) - |\nabla\Phi(x)|^2) e^{2\Phi(x)/h}|u(x)|^2 dx \\ &= \operatorname{Re} \int_\Omega e^{2\Phi(x)/h} Pu(x)\overline{u}(x) dx. \end{aligned} \tag{2.1}$$

Here $|\cdot|$ denotes the standard norm on scalars or vectors. In the Riemannian case the norm of the gradient is the natural one for cotangent vectors. Δ denotes the Laplace-Beltrami operator and dx is the natural volume element.

Proposition 6.2 in [3] extends to:

Proposition 2.2.— *Under the assumptions of Proposition 2.1, let $0 \leq F_\pm \in L^\infty(\Omega)$ and $\Phi \in \mathcal{C}^2(\overline{\Omega};\mathbb{R})$ satisfy*

$$\operatorname{Re} V - (\nabla\Phi(x))^2 = F_+(x)^2 - F_-(x)^2 \text{ almost everywhere.}$$

Then

$$h^2\|\nabla(e^{\Phi/h}u)\|^2 + \frac{1}{2}\|F_+e^{\Phi/h}u\|^2 \leq \|\frac{1}{F_+ + F_-}e^{\Phi/h}Pu\|^2 + \frac{3}{2}\|F_-e^{\Phi/h}u\|^2.$$

The propositions 2.1, 2.2 allow us to make an immediate extension of the discussion of the Lithner-Agmon (that we abbreviate with LA) metric (originally introduced in [5] and [1]) and Proposition 6.4 in [3]. We just have to replace the real potential there by the real

part V_0 of the potential V_ε and recall that we work near the real energy level 0. We repeat the discussion for completeness.

The LA metric is defined to be

$$V_0(x)_+ dx^2. \tag{2.2}$$

For a $\mathcal{C}^1$ curve γ we let $|\gamma|$ denote its length in the LA-metric. If $x, y \in M$ we define the LA distance $d(x,y)$ between x and y to be the infimum of the lengths $|\gamma|$ for all $\mathcal{C}^1$ curves from y to x. This distance may be degenerate in the sense that we may have $d(x,y) = 0$ for distinct points x and y. Nevertheless:

$$d(x,y) = d(y,x),\ d(x,z) \leq d(x,y) + d(y,z), \tag{2.3}$$

$$|d(x,z) - d(x,y)| \leq d(y,z). \tag{2.4}$$

Further, $y \mapsto d(x,y)$ is a locally Lipschitz function and

$$|d(x,z) - d(x,y)| \leq (V_0(y)_+ + o(1))^{\frac{1}{2}} |z-y|_y, \tag{2.5}$$

when $z \to y$, where $|.|_y$ is the Riemannian norm on T_yM and we identify $\operatorname{neigh}(0, T_yM)$ with $\operatorname{neigh}(y, M)$ by means of the exponential map. It follows that for all $x, y \in M$,

$$|\nabla_y d(x,y)| \leq V_0(y)_+^{\frac{1}{2}}, \tag{2.6}$$

$$|\nabla_x d(x,y)| \leq V_0(x)_+^{\frac{1}{2}}. \tag{2.7}$$

If $U \subset M$, we put $d(x,U) = \inf_{y\in U} d(x,y)$. Then $|d(x,U) - d(y,U)| \leq d(x,y)$, so $|\nabla_x d(x,U)| \leq V_0(x)_+^{\frac{1}{2}}$ a.e. on M.

Proposition 6.4 in [3] remains valid, but we prefer to give the following variant whose proof is basically the same:

Proposition 2.3.— *Let $\mathcal{E} \subset \mathbb{R}$, $K \subset M$ be compact sets, $0 < h_0 << 1$ and assume that*

$$(P_\varepsilon - z)u = v, \quad z = z(h) \to 0 \text{ as } h \to 0$$

where $\varepsilon = \varepsilon(h) \in \mathcal{E}$, $u = u(h) \in \mathcal{D}(P_0)$, $v = v(h) \in L^2$, $\operatorname{supp} v \subset K$. Then for every fixed $\delta > 0$ there exists a constant C_δ (independent of u, v) such that

$$\|\nabla(e^{(1-\delta)\widetilde{\Phi}/h}u)\| + \|e^{(1-\delta)\widetilde{\Phi}/h}(1 + V_{0+}^{\frac{1}{2}})u\| \leq C_\delta e^{\delta/h} \|u\|_{H^1(K_\delta)},$$

where

$$K_\delta = \{x \in M;\ d_M(x,K) < \delta\},\ \widetilde{\Phi}(x) = d(U,x).$$

Here d_M denotes the Riemannian distance.

We end this section by recalling some terminology from [3] (earlier used in the works of Helffer and Sjöstrand, cf. [4]). Let $A = A_h$ be a family of operators $L^2(M) \to H^1(M)$ depending on $h \in]0, h_0[$ where $h_0 > 0$ is small. Let $f \in C^0(M \times M; \mathbb{R})$. We say that the kernel $A(x,y)$ of A (using the same notation for an operator and its distribution kernel)

is $\widehat{\mathcal{O}}(e^{-f(x,y)/h})$ if for all $x_0, y_0 \in M$ and $\delta > 0$, there exist neighborhoods $V, U \subset M$ of x_0 and y_0 and a constant $C > 0$, such that

$$\|Au\|_{H^1(V)} \leq Ce^{-(f(x_0,y_0)-\delta)/h}\|u\|_{L^2(U)}$$

for all $u \in L^2(M)$ with support in U. We have the analogous definitions for operators $L^2(M) \to L^2(M)$ and the choice of arrival space will be clear from the context. If not, we write $\widehat{\mathcal{O}}_{L^2\to H^1}(e^{-f/h})$ and $\widehat{\mathcal{O}}_{L^2\to L^2}(e^{-f/h})$, to specify.

We make two observations in the case when M is compact

1) If $A(x,y) = \widehat{\mathcal{O}}_{L^2\to X}(e^{-f/h})$, $B(x,y) = \widehat{\mathcal{O}}_{L^2\to L^2}(e^{-g/h})$, where X is equal to L^2 or H^1, then $A \circ B(x,y) = \widehat{\mathcal{O}}_{L^2\to X}(e^{-k/h})$, where $k(x,y) = \min_{x\in M}(f(x,z) + g(z,y))$.
2) There is an obviously analogous notion $u = \widehat{\mathcal{O}}_X(e^{\phi(x)/h})$ when $\phi \in \mathcal{C}(M;\mathbb{R})$, $u \in X$, $X = L^2$ or $X = H^1$. Let $A(x,y) = \widehat{\mathcal{O}}_{L^2\to X}(e^{-f(x,y)/h})$, $u = \widehat{\mathcal{O}}_{L^2}(e^{\phi/h})$ where $\phi \in \mathcal{C}(M;\mathbb{R})$. Then, $Au = \widehat{\mathcal{O}}_X(e^{\psi/h})$, where $\psi(x) = \sup_{y\in M}(-k(x,y) + \phi(y))$.

When $M = \mathbb{R}^n$, one can adapt these notions provided that we have some uniform exponential decay near infinity. Below, we will always be in such situations, so we shall proceed as in the compact case.

3. Proof of the main result

Let $\widetilde{e}_j = \widetilde{e}_j(h)$ be normalized eigenfunctions of $\widetilde{P}_j$ corresponding to the eigenvalue $\mu(h)$:

$$(\widetilde{P}_j - \widetilde{\mu})\widetilde{e}_j = 0. \tag{3.1}$$

We choose $\widetilde{e}_j$ so that

$$\mathcal{P}\widetilde{e}_j = \widetilde{e}_{-j}. \tag{3.2}$$

We know that

$$\widetilde{e}_j = \widehat{\mathcal{O}}_{H^1}(e^{-d(U_j,x)/h}), \tag{3.3}$$

and we have nice uniform exponential decay estimates near infinity when $M = \mathbb{R}^n$ (cf. Proposition 2.2). In particular,

$$(\widetilde{e}_1|\widetilde{e}_{-1}) = \widehat{\mathcal{O}}(e^{-S_0/h}), \tag{3.4}$$

where we extended the notion $\widehat{\mathcal{O}}$ to scalar quantities in the natural way.

We know that for h small enough, the spectrum of P_0 in

$$]\widetilde{\mu} - \frac{h^{N_0}}{2C_0}, \widetilde{\mu} + \frac{h^{N_0}}{2C_0}[\tag{3.5}$$

consists of two simple or one double double eigenvalue. Let $\mathcal{E}_0(h) \subset L^2(M)$ be the corresponding 2-dimensional spectral subspace and let $\Pi_0(h) : L^2(M) \to L^2(M)$ be the associated spectral projection. Since P_0 is self-adjoint, we know that Π_0 is orthogonal, $\Pi_0 = \Pi_0^*$.

The functions $\Pi_0\widetilde{e}_j$, $j = \pm 1$ form a basis in $\mathcal{E}_0(h)$ and we have

$$\Pi_0\widetilde{e}_j(x) - \widetilde{e}_j(x) = \widehat{\mathcal{O}}(e^{-\frac{1}{h}(d(U^\delta_{-j},x)+S_0-2\delta)}). \tag{3.6}$$

From (3.4) we see that $\Pi_0\widetilde{e}_j$ form an almost orthonormal basis in $\mathcal{E}_0(h)$ (see [3] for more details) and this basis can be orthonomalized by using the square root of the Gram matrix (which is very close to the idenity) in order to produce an orthonormal basis e_1, e_{-1} such that

$$e_j - \widetilde{e}_j = \widetilde{\mathcal{O}}(e^{-\frac{1}{h}(S_0+d(U_{-j},x))}) \tag{3.7}$$

where we use the notation $\widetilde{\mathcal{O}}(e^{f/h})$ for $\mathcal{O}(e^{(f-\varepsilon(\delta))/h})$ (or $\widehat{\mathcal{O}}(e^{(f-\varepsilon(\delta))/h})$ depending on the context) for every fixed $\delta > 0$, where $\varepsilon(\delta) \to 0$ when $\delta \to 0$. The matrix of $P_{0|_{\mathcal{E}_0(h)}}$ with respect to this basis is

$$\begin{pmatrix} \mu(h) & t(h) \\ \overline{t(h)} & \mu(h) \end{pmatrix}, \tag{3.8}$$

where

$$\mu(h) = \widetilde{\mu}(h) + \widetilde{\mathcal{O}}(e^{-2S_0/h}) \tag{3.9}$$

is real and the tunneling coefficient fulfills

$$t(h) = \widehat{\mathcal{O}}(e^{-S_0/h}). \tag{3.10}$$

See Theorem 6.10 in [3].

In many situation we have a matching lower bound on $|t(h)|$:

$$1/|t(h)| = \widehat{\mathcal{O}}(e^{S_0/h}). \tag{3.11}$$

The two eigenvalues of $P_0(h)$ in the interval (3.5) are the ones of the matrix (3.8):

$$\mu_{\pm 1}(h) = \mu(h) \pm |t(h)|. \tag{3.12}$$

We now turn to the perturbed operator P_ε, where $W \in \mathcal{C}^\infty(M;\mathbb{R}) \cap L^\infty(M)$ and we assume for simplicity, that $\|W\|_{L^\infty} \leq 1$. As for ε, we require that

$$|\varepsilon| \ll h^{N_0}. \tag{3.13}$$

We know that the spectrum of P_ε is discrete in some fixed (h-independent) neighborhood of 0 when h and $|\varepsilon|$ are small enough. From the assumption (3.13), it follows that P_ε has precisely two eigenvalues, counted with their (algebraic) multiplicity, in the disc $D(\widetilde{\mu}, h^{N_0}/(2C))$ and these eigenvalues belong to the smaller disc $D(\mu(h), |t(h)| + \varepsilon)$. Let

$\mathcal{E}_\varepsilon(h)$ be the corresponding 2-dimensional spectral subspace and let $\Pi_\varepsilon(h) : L^2(M) \to \mathcal{E}_\varepsilon(h)$ be the spectral projection, where we recall the Riesz formula

$$\Pi_\varepsilon = \frac{1}{2\pi i}\int_\gamma (z-P_\varepsilon)^{-1}dz,\ \gamma = \partial D(\widetilde{\mu}, \frac{h^{N_0}}{2C}). \tag{3.14}$$

Here $D(z_0, r)$ denotes the open disc in $\mathbb{C}$ of center z_0 and radius r. Using the Riesz formula (cf. [3, p.62]) we obtain

$$\|\Pi_\varepsilon - \Pi_0\| = \mathcal{O}(\varepsilon h^{-N_0}) \ll 1. \tag{3.15}$$

Thus, introducing

$$e_j^\varepsilon = \Pi_\varepsilon e_j, \tag{3.16}$$

we see that e_1^ε, e_{-1}^ε form a basis for $\mathcal{E}_\varepsilon(h)$ which is close to be orthonormal. Differentiating in (3.14), we see that

$$\partial_\varepsilon \Pi_\varepsilon = \mathcal{O}(h^{-N}), \tag{3.17}$$

which also implies (3.15).

As we have seen in Section 2, LA estimates work also for P_ε and we have

$$e_j^\varepsilon,\ \partial_\varepsilon e_j^\varepsilon = \widetilde{\mathcal{O}}(e^{-d(U_j,x)/h}). \tag{3.18}$$

In fact, we know as in the self-adjoint case ([3]) that Π_ε, $\partial_\varepsilon\Pi_\varepsilon = \widehat{\mathcal{O}}(e^{-d(x,y)/h})$ and $e_j = \mathcal{O}(e^{-d(U_j,x)/h})$. The functions e_j^ε, $j=\pm 1$, form an orthonormal basis for $\mathcal{E}_\varepsilon(h)$ when $\varepsilon = 0$ but not necessarily when $\varepsilon \neq 0$. Recalling that $P_\varepsilon^* = P_{-\varepsilon}$, we let $f_1^\varepsilon, f_{-1}^\varepsilon \in \mathcal{E}_{-\varepsilon}(h)$ be the dual basis to e_1^ε, $\varepsilon_{-1}^\varepsilon \in \mathcal{E}_\varepsilon(h)$:

$$(f_j^\varepsilon | e_k^\varepsilon) = \delta_{j,k},\ j,k \in \{-1,1\}. \tag{3.19}$$

Proposition 3.1.— *We have*

$$f_k^\varepsilon,\ \partial_\varepsilon f_k^\varepsilon = \widetilde{\mathcal{O}}(e^{-d(U_k,x)/h}),\ k=\pm 1. \tag{3.20}$$

Proof. Let $b_{j,k} = (e_j^{-\varepsilon} | e_k^\varepsilon)$, so that in the space of 2×2-matrices,

$$(b_{j,k}) = 1 + \mathcal{O}(\varepsilon h^{-N_0}) \tag{3.21}$$

by (3.15). By (3.18) we have

$$b_{j,k},\ \partial_\varepsilon b_{j,k} = \widetilde{\mathcal{O}}(e^{-S_0/h}),\ \text{when } j \neq k. \tag{3.22}$$

Write

$$f_j^\varepsilon = \sum_\nu c_{j,\nu} e_\nu^{-\varepsilon}.$$

Then (3.19) reads

$$\sum_\nu c_{j,\nu}(e_\nu^{-\varepsilon} | e_k^\varepsilon) = \delta_{j,k},$$

i.e.

$$\sum_\nu c_{j,\nu} b_{\nu,k} = \delta_{j,k},$$

so

$$(c_{j,k}) = (b_{j,k})^{-1} = \begin{pmatrix} 1/b_{1,1} & 0 \\ 0 & 1/b_{-1,-1} \end{pmatrix} + \widetilde{\mathcal{O}}(e^{-S_0/h}),\ b_{j,j} = 1 + \mathcal{O}(\varepsilon h^{-N_0}), \tag{3.23}$$

where the last equality follows from (3.21). We therefore get the estimate for f_k^ε in (3.20).

In order to get the estimate for $\partial_\varepsilon f_k^\varepsilon$ in (3.20), we first observe that

$$\partial_\varepsilon b_{j,j} = \mathcal{O}(h^{-N_0}),\ \partial_\varepsilon b_{j,k} = \widetilde{\mathcal{O}}(e^{-S_0/h}),\ \text{when } j \neq k. \tag{3.24}$$

Combining this with the standard formula

$$\partial_\varepsilon (c_{j,k}) = -(c_{j,k}) \circ \partial_\varepsilon (b_{j,k}) \circ (c_{j,k}),$$

(3.21) and (3.23), we see that $c_{j,k}$ also satisfy (3.24):

$$\partial_\varepsilon c_{j,j} = \mathcal{O}(h^{-N_0}),\ \partial_\varepsilon c_{j,k} = \widetilde{\mathcal{O}}(e^{-S_0/h}),\ \text{when } j \neq k. \tag{3.25}$$

Now,

$$\partial_\varepsilon f_k^\varepsilon = \sum_\nu (\partial_\varepsilon c_{k,\nu}) e_\nu^{-\varepsilon} + \sum_\nu c_{k,\nu} (\partial_\varepsilon e_\nu^{-\varepsilon})$$

and the estimate for $\partial_\varepsilon f_k^\varepsilon$ in (3.20) follows from (3.21), (3.23), (3.18) with ε replaced by $-\varepsilon$ in the last relation. $\square$

Let $M_\varepsilon = (m_{j,k}^\varepsilon)$ denote the matrix of $P_\varepsilon = \mathcal{E}_\varepsilon(h) \to \mathcal{E}_\varepsilon(h)$ with respect to the basis e_1^ε, e_{-1}^ε. Then

$$m_{j,k}^\varepsilon = (P_\varepsilon e_k^\varepsilon | f_j^\varepsilon) = (e_k^\varepsilon | P_{-\varepsilon} f_j^\varepsilon). \tag{3.26}$$

Note that $f_j^0 = e_j^0$ since e_1^0, e_{-1}^0 is an orthonormal basis, and that M_0 is the matrix in (3.8).

Naturally, the $\mathcal{PT}$-symmetry of P_ε induces a corresponding symmetry for M_ε that we shall make explicit. By construction, we have $\mathcal{PT} e_j^\varepsilon = e_{-j}^\varepsilon$. Also notice that

$$(\mathcal{PT} u | \mathcal{PT} v) = \overline{(u|v)} = (v|u),\ u, v \in L^2(M).$$

From (3.19), we get

$$(\mathcal{PT} f_j^\varepsilon | \mathcal{PT} e_k^\varepsilon) = \delta_{j,k},$$

i.e.

$$(\mathcal{PT} f_j^\varepsilon | e_{-k}^\varepsilon) = \delta_{j,k} = \delta_{-j,-k}.$$

Comparing with (3.19) (and recalling that $\mathcal{E}_\varepsilon$ and $\mathcal{E}_{-\varepsilon}$ are invariant under the action of $\mathcal{PT}$) we conclude that

$$\mathcal{PT} f_j^\varepsilon = f_{-j}^\varepsilon. \tag{3.27}$$

We have,

$$\begin{aligned} m^{\varepsilon}_{j,k} &= (P_\varepsilon e^{\varepsilon}_k | f^{\varepsilon}_j) = (P_\varepsilon \mathcal{PT} e^{\varepsilon}_{-k} | \mathcal{PT} f^{\varepsilon}_{-j}) \\ &= (\mathcal{PT} P_\varepsilon e^{\varepsilon}_{-k} | \mathcal{PT} f^{\varepsilon}_{-j}) = \overline{(P_\varepsilon e^{\varepsilon}_{-k} | f^{\varepsilon}_{-j})} = \overline{m^{\varepsilon}_{-j,-k}}, \end{aligned} \tag{3.28}$$

which means that the general form of M_ε is

$$M_\varepsilon = \begin{pmatrix} a(\varepsilon) & b(\varepsilon) \\ \overline{b}(\varepsilon) & \overline{a}(\varepsilon) \end{pmatrix}. \tag{3.29}$$

This can also be expressed as a $\mathcal{PT}$-symmetry property of M_ε as a linear map: $\mathbb{C}^2 \to \mathbb{C}^2$: Define $\pi, \tau : \mathbb{C}^2 \to \mathbb{C}^2$ by

$$\pi \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_2 \\ x_1 \end{pmatrix}, \quad \tau \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \overline{x}_1 \\ \overline{x}_2 \end{pmatrix}. \tag{3.30}$$

Then (3.28) is equivalent to the property,

$$\pi \tau M_\varepsilon = M_\varepsilon \pi \tau. \tag{3.31}$$

Since this formulation will not be needed below, we leave out the simple and straight forward proof.

We now study $\partial_\varepsilon m^{\varepsilon}_{j,k}$. First, if $j \neq k$, we have

$$\partial_\varepsilon m^{\varepsilon}_{j,k} = i(W e^{\varepsilon}_k | f^{\varepsilon}_j) + (P_\varepsilon \partial_\varepsilon e^{\varepsilon}_k | f^{\varepsilon}_j) + (P_\varepsilon e^{\varepsilon}_k | \partial_\varepsilon f^{\varepsilon}_j) = \widetilde{\mathcal{O}}(e^{-S_0/h}). \tag{3.32}$$

For $j = k$, we start with

$$\partial_\varepsilon m^{\varepsilon}_{j,j} = i(W e^{\varepsilon}_j | f^{\varepsilon}_j) + (P_\varepsilon \partial_\varepsilon e^{\varepsilon}_j | f^{\varepsilon}_j) + (P_\varepsilon e^{\varepsilon}_j | \partial_\varepsilon f^{\varepsilon}_j). \tag{3.33}$$

Here we use that $e^{\varepsilon}_j = e^0_j + \mathcal{O}(\varepsilon h^{-N_0})$, $f^{\varepsilon}_j = f^0_j + \mathcal{O}(\varepsilon h^{-N_0})$ in L^2, to see that

$$(W e^{\varepsilon}_j | f^{\varepsilon}_j) = (W e^0_j | e^0_j) + \mathcal{O}(\varepsilon h^{-N_0}) = \int W(x) |e^0_j(x)|^2 dx + \mathcal{O}(\varepsilon h^{-N_0}). \tag{3.34}$$

In order to treat the other two terms in (3.33), we recall that by definition of $m^{\varepsilon}_{j,k}$, we have

$$P_\varepsilon e^{\varepsilon}_j = \sum_\nu m^{\varepsilon}_{\nu,j} e^{\varepsilon}_\nu. \tag{3.35}$$

We need a similar formula for $P^*_\varepsilon f^{\varepsilon}_j$, so we take the L^2 inner product of (3.35) with f^{ε}_k and get

$$(e^{\varepsilon}_j | P^*_\varepsilon f^{\varepsilon}_k) = \sum_\nu m^{\varepsilon}_{\nu,j} \underbrace{(e^{\varepsilon}_\nu | f^{\varepsilon}_k)}_{\delta_{\nu,k}} = m^{\varepsilon}_{k,j}.$$

Exchange j, k and take the complex conjugates:

$$(P^*_\varepsilon f^{\varepsilon}_j | e^{\varepsilon}_k) = \overline{m}^{\varepsilon}_{j,k},$$

to conclude that

$$P^*_\varepsilon f^{\varepsilon}_j = \sum_\nu \overline{m}^{\varepsilon}_{j,\nu} f^{\varepsilon}_\nu. \tag{3.36}$$

Using (3.35), (3.36), we get

$$\begin{aligned}(P_\varepsilon\partial_\varepsilon e_j^\varepsilon|f_j^\varepsilon)+(P_\varepsilon e_j^\varepsilon|\partial_\varepsilon f_j^\varepsilon)&=(\partial_\varepsilon e_j^\varepsilon|P_\varepsilon^* f_j^\varepsilon)+(P_\varepsilon e_j^\varepsilon|\partial_\varepsilon f_j^\varepsilon)\\&=\sum_\nu\left(m_{j,\nu}^\varepsilon(\partial_\varepsilon e_j^\varepsilon|f_\nu^\varepsilon)+m_{\nu,j}^\varepsilon(e_\nu^\varepsilon|\partial_\varepsilon f_j^\varepsilon)\right)\\&=m_{j,j}^\varepsilon\underbrace{\left((\partial_\varepsilon e_j^\varepsilon|f_j^\varepsilon)+(e_j^\varepsilon|\partial_\varepsilon f_j^\varepsilon)\right)}_{\partial_\varepsilon(e_j^\varepsilon|f_j^\varepsilon)=\partial_\varepsilon(1)=0}\\&\qquad+\underbrace{m_{j,-j}^\varepsilon}_{\widetilde{\mathcal{O}}(e^{-S_0/h})}\underbrace{(\partial_\varepsilon e_j^\varepsilon|f_{-j}^\varepsilon)}_{\widetilde{\mathcal{O}}(e^{-S_0/h})}+\underbrace{m_{-j,j}^\varepsilon}_{\widetilde{\mathcal{O}}(e^{-S_0/h})}\underbrace{(e_{-j}^\varepsilon|\partial_\varepsilon f_j^\varepsilon)}_{\widetilde{\mathcal{O}}(e^{-S_0/h})}\\&=\widetilde{\mathcal{O}}(e^{-2S_0/h}).\end{aligned}$$

Combining this with (3.33), (3.34), we obtain

$$\partial_\varepsilon m_{j,j}^\varepsilon=i\int W(x)|e_j^0(x)|^2dx+\mathcal{O}(\varepsilon h^{-N_0})+\widetilde{\mathcal{O}}(e^{-2S_0/h}) \tag{3.37}$$

and by integration in ε (cf. (3.29), (3.8)),

$$a(\varepsilon)=\mu(h)+i\varepsilon\int W(x)|e_j^\varepsilon(x)|^2dx+\mathcal{O}(\varepsilon^2h^{-N_0})+\varepsilon\widetilde{\mathcal{O}}(e^{-2S_0/h}). \tag{3.38}$$

By (3.32), we have

$$\partial_\varepsilon b,\ \partial_\varepsilon|b|=\widetilde{\mathcal{O}}(e^{-S_0/h}), \tag{3.39}$$

which implies that

$$b(\varepsilon)=t(h)+\varepsilon\widetilde{\mathcal{O}}(e^{-S_0/h}). \tag{3.40}$$

The eigenvalues of $P_{\varepsilon|_{\mathcal{E}_\varepsilon(h)}}$ are equal to the ones of M_ε (cf. (3.29)):

$$\lambda_\pm=\operatorname{Re}a\pm\sqrt{|b|^2-(\operatorname{Im}a)^2}. \tag{3.41}$$

Assume now that

$$W>0 \text{ on } U_1 \tag{3.42}$$

and hence also on a fixed neighborhood of that set. Since e_1^0 is exponentially concentrated to a neighborhood of U_1, we conclude that

$$\int W(x)|e_1^0(x)|^2dx\asymp 1, \tag{3.43}$$

and (3.37) shows that

$$\partial_\varepsilon\operatorname{Im}a=\int W|e_1^0|^2dx+\mathcal{O}(\varepsilon h^{-N_0})+\widetilde{\mathcal{O}}(e^{-2S_0/h})\asymp 1. \tag{3.44}$$

We can now discuss when the two eigenvalues (cf. (3.41)) are real or complex. Since we are dealing with a $\mathcal{PT}$ symmetric operator, we know that the eigenvalues are either real or form complex conjugate pairs. This means that $P_{-\varepsilon} = P_\varepsilon^*$ and P_ε have the same spectrum. Consequently, we can restrict the attention to the region $0 \le \varepsilon \ll h^{N_0}$. The reality or not of our two eigenvalues is determined by the sign of

$$|b| - (\operatorname{Im} a)^2 = (|b| + \operatorname{Im} a)(|b| - \operatorname{Im} a). \tag{3.45}$$

Recall that $\operatorname{Im} a$ vanishes when $\varepsilon = 0$ and is a strictly increasing function of ε whose derivative is $\asymp 1$, while $b(\varepsilon)$ and its derivative with respect to ε are exponentially small. Thus, if we first consider the case when $t(h) = 0$, we see that both factors in (3.45) vanish for $\varepsilon = 0$ (corresponding to a double real eigenvalue of P_0) and for $\varepsilon > 0$ the first factor is positive while the second one is negative, so the two eigenvalues in (3.41) are non-real and complex conjugate for $\varepsilon > 0$.

Let now $t(h) \neq 0$ (but still exponentially small as we recalled in (3.10)). Then the first factor in (3.45) is strictly positive for $0 \le \varepsilon \ll h^{N_0}$. Denote the second factor by $f(\varepsilon) = |b| - \operatorname{Im} a$. Then $f(0) = |t(h)| > 0$ and

$$f'(\varepsilon) = -\int W(x)|e_j^0|^2 dx + \mathcal{O}(\varepsilon h^{-N_0}) + \widetilde{\mathcal{O}}(e^{-S_0/h}) \asymp -1. \tag{3.46}$$

Hence there exists a point $\varepsilon_+(h) > 0$ such that $f(\varepsilon) > 0$ for $0 \le \varepsilon < \varepsilon_+$, $f(\varepsilon_+) = 0$, $f(\varepsilon) < 0$ for $e_+ < \varepsilon \ll h^{N_0}$. In the first region we have two real and distinct eigenvalues, at the point ε_+ we have a real double eigenvalue, while in the last region we have a pair of complex conjugate non-real eigenvalues.

In view of (3.10) and (3.46) we know that $\varepsilon_+(h) = \widehat{\mathcal{O}}(e^{-S_0/h})$ and if we restrict the attention to the exponentially small interval $[0, 2\varepsilon_+]$ we can sharpen (3.46) to

$$f'(\varepsilon) = -\int W(x)|e_j^0(x)|^2 dx + \widetilde{\mathcal{O}}(e^{-S_0/h}),$$

which implies that

$$\varepsilon_+ = (1 + \widetilde{\mathcal{O}}(e^{-S_0/h}))\frac{|t(h)|}{\int W(x)|e_1^0(x)|^2 dx}, \tag{3.47}$$

and this finishes the proof of Theorem 1.1.

Appendix A. The spectrum of P_ε

We recall from the Introduction that P_0 denotes the Friedrichs extension of the differential operator $-h^2\Delta + V_0$ from $\mathcal{C}_0^\infty(M)$, $M = \mathbb{R}^n$ or a Riemannian compact manifold. In the first case

$$\alpha = \liminf_{x\to\infty} V_0(x),$$

and $\alpha = +\infty$ in the latter case. We recall that the domain $\mathcal{D}(P_0)$ of P_0 contains the form domain

$$\{u \in L^2(M);\ \int |\nabla u|^2 dx + \int (V_0)_+(x)|u|^2 dx < +\infty\},$$

where $(V_0)_+(x) = \max(V_0(x), 0)$.

Proposition A.1.— *The spectrum of P_ε in the left half-plane* $\operatorname{Re} z < \alpha$ *is discrete.*

Proof. When M is compact this follows quite easily from the ellipticity of P_ε and the fact that there are always points with $\operatorname{Re} z \ll 0$ that do not belong to the spectrum.

Thus, we consider the case when $M = \mathbb{R}^n$. Let $\beta < \alpha$ be arbitrarily close to α and put $V_{0,\beta}(x) = \max(V_0(x), \beta)$ so that $V_{0,\beta}$ is equal to V_0 near infinity or equivalently so that $\operatorname{supp}(V_{0,\beta} - V_0)$ is compact. Put $P_{\varepsilon,\beta} = -h^2\Delta + V_{0,\beta}(x) + i\varepsilon W(x)$.

Let us first notice that $P_{\varepsilon,\beta} - z : \mathcal{D}(P_0) \to L^2$ is bijective with bounded inverse when $\operatorname{Re} z < \beta$. Indeed, the injectivity follows from the estimate

$$\operatorname{Re}((P_{\varepsilon,\beta} - z)u|u) \geq ((V_{0,\beta} - \operatorname{Re} z)u|u) \geq (\beta - \operatorname{Re} z)\|u\|^2,\ u \in \mathcal{D}(P_0).$$

Notice also from this that $P_{\varepsilon,\beta} - z$ has a bounded left inverse $R_{\varepsilon,\beta}(z)$ of norm $\leq (\beta - \operatorname{Re} z)^{-1}$ in $\mathcal{L}(L^2, L^2)$. When $\varepsilon = 0$, $P_{0,\beta}$ is self-adjoint and $P_{0,\beta} - z$ is bijective, so the left inverse is a bilateral inverse. By a simple deformation argument in ε we get the claimed bijectivity for all ε.

Still for $\operatorname{Re} z < \beta$ we write

$$P_\varepsilon - z = P_{\varepsilon,\beta} - z + (V_0 - V_{0,\beta}) = \begin{cases} (P_{\varepsilon,\beta} - z)(1 + (P_{\varepsilon,\beta} - z)^{-1}(V_0 - V_{0,\beta})) \\ \text{and also} \\ (1 + (V_0 - V_{0,\beta})(P_{\varepsilon,\beta} - z)^{-1})(P_{\varepsilon,\beta} - z). \end{cases}$$

Here $(V_0 - V_{0,\beta}) : \mathcal{D}(P_0) \to L^2$ is compact, since $V_0 - V_{0,\beta} \in L^\infty_{\text{comp}}$, so

$$\begin{aligned} &(P_{\varepsilon,\beta} - z)^{-1}(V_0 - V_{0,\beta}) :\ \mathcal{D}(P_0) \to \mathcal{D}(P_0), \\ &(V_0 - V_{0,\beta})(P_{\varepsilon,\beta} - z)^{-1} :\ L^2 \to L^2 \end{aligned}$$

are compact. The operator norms of these operators are $\mathcal{O}((\beta - \operatorname{Re} z)^{-1})$. Thus

$$1 + (P_{\varepsilon,\beta} - z)^{-1}(V_0 - V_{0,\beta}) :\ \mathcal{D}(P_0) \to \mathcal{D}(P_0)$$

and

$$1 + (V_0 - V_{0,\beta})(P_{\varepsilon,\beta} - z)^{-1} :\ L^2 \to L^2$$

are holomorphic families of Fredholm operators of index 0, bijective when $\operatorname{Re} z \ll 0$. From these observations we get the proposition in a fairly standard way. $\square$

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